Figure 1

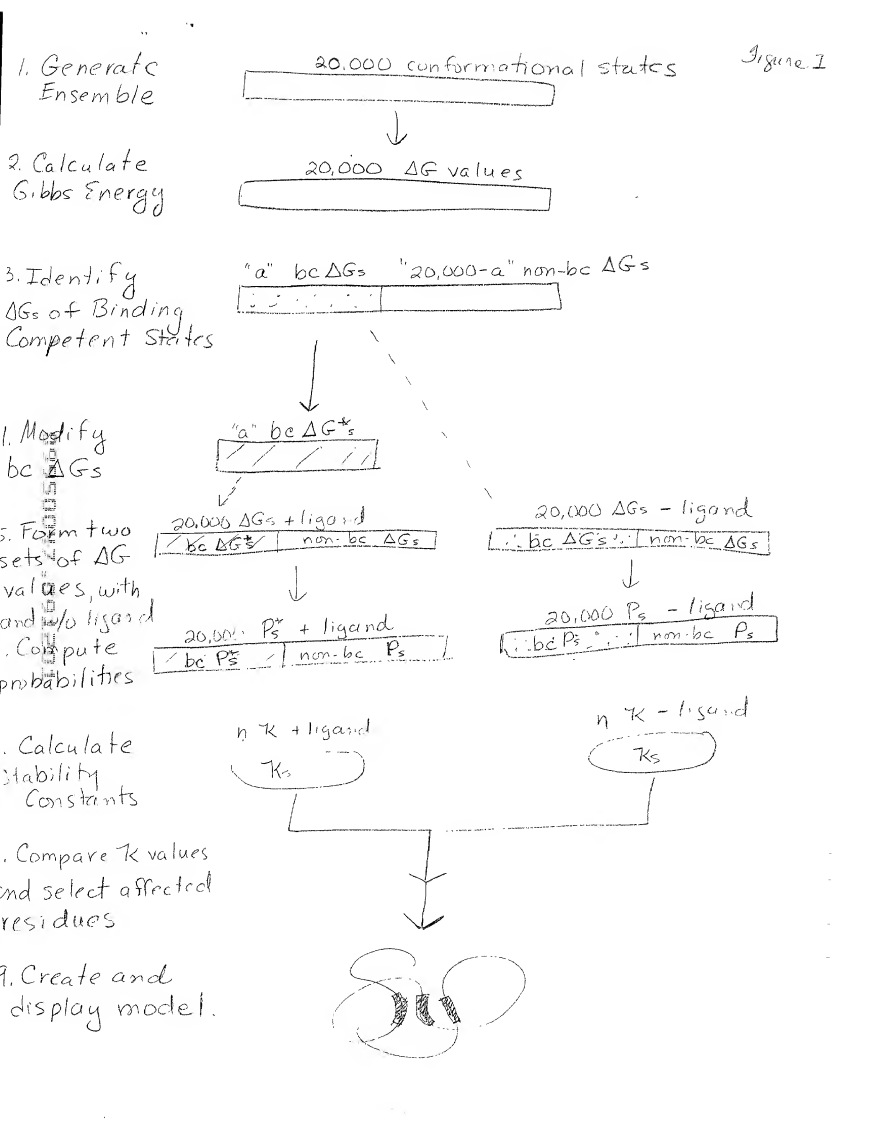
1. Generate Ensemble
20,000 conformational states
2. Calculate Gibbs Energy
20,000 ΔG values
3. Identify ΔGs of Binding Competent States
"a" bc ΔGs
"20,000-a" non-bc ΔGs
4. Modify bc ΔGs
"a" bc ΔG*s
5. Form two sets of ΔG values, with and w/o ligand
20,000 ΔGs + ligand
bc ΔG*s
non-bc ΔGs
20,000 ΔGs - ligand
bc ΔGs
non-bc ΔGs
6. Compute probabilities
20,000 P*s + ligand
bc P*s
non-bc Ps
20,000 Ps - ligand
bc Ps
non-bc Ps
7. Calculate Stability Constants
n K + ligand
Ks
n K - ligand
Ks
8. Compare K values and select affected residues
9. Create and display model.

Figure 2

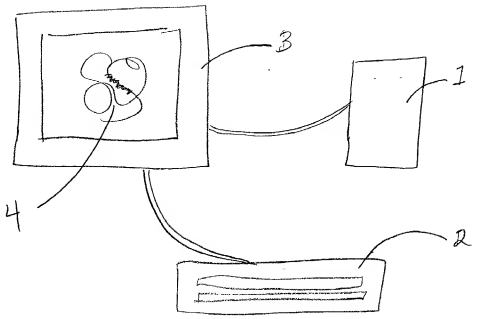

Figure 3